A RELAXATION METHOD FOR THE COMPUTATION OF MODEL STELLAR ATMOSPHERES*

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Abstract. A general Monte Carlo relaxation method has been formulated for the computation of physically self-consistent model stellar atmospheres. The local physical state is obtained by solving simultaneously the equations of statistical equilibrium for the atomic and ionic level populations, the kinetic energy balance equation for the electron gas to obtain the electron temperature, and the equation of radiative transfer. Anisotropic Thomson scattering is included in the equation of transfer and radiation pressure effects are included in the hydrostatic equation. The constraints of hydrostatic and radiative equilibrium are enforced. Local thermodynamic equilibrium (L.T.E.) is assumed as a boundary condition deep in the atmosphere. Elsewhere in the atmosphere L.T.E. is not assumed.

The statistical equilibrium equations are solved with no assumptions made concerning detailed balance for the bound-bound radiative processes. The source function is formulated in microscopic detail. All atomic processes contributing to the absorption and emission of radiation are included. The kinetic energy balance equation for the electron gas is formulated in detail. All atomic processes by which kinetic energy is gained and lost by the electron gas are included.

The method has been applied to the computation of a model atmosphere for a pure hydrogen early-type star. An idealized model of the hydrogen atom with five bound levels and the continuum was adopted. The results of the trial calculation are discussed with reference to stability, accuracy, and convergence of the solution.

1. Introduction

Much progress has been made during the last decade in developing methods for the computation of model stellar atmospheres. Methods currently in use have been reviewed recently in detail by MIHALAS (1967a). These methods were developed specifically for atmospheres which are assumed to be in hydrostatic and radiative equilibrium throughout. Local thermodynamic equilibrium (L.T.E.) is assumed everywhere in the atmosphere and the atomic and ionic level populations are obtained from the Boltzmann and Saha equations for the local temperature. The source function is assumed to be the sum of two terms, a thermal term and an electron-scattering term. The former is represented by the Planck function at the local temperature, while the latter depends on the intensity of the radiation field averaged over all solid angles. The local temperature is obtained by determining that temperature required for the Planck term of the source function to maintain radiative equilibrium. These methods have reached a high level of mathematical accuracy. Rapidly convergent iterative procedures now exist for obtaining the temperature as a function of optical depth. The condition of radiative equilibrium can be stringently applied with the

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net outward flux, integrated over wavelength, held constant with optical depth to a small fraction of 1%. Recently KALKOFEN (1966), STROM and KALKOFEN (1966a, b), STROM (1967), and MIHALAS (1967b, c, 1968) have extended these methods by relaxing the assumption of L.T.E. In their work the atomic level populations and source function are coupled to the radiation field. The statistical equilibrium equations are solved with the assumption of detailed balance for the bound-bound radiative processes. Elimination of the latter assumption is crucial for the further development of stellar atmosphere theory.

In this paper a novel method for the computation of model stellar atmospheres is described. Fundamental simplicity has been emphasized in the formulation of the method and the algorithm is closely associated with the basic physics of a stellar atmosphere.

In the new method the equations of statistical equilibrium for each atom, the kinetic energy balance equation for the electron gas, and the equation of radiative transfer are solved simultaneously. The atomic and ionic level populations are obtained from the statistical equilibrium equations, while the local electron temperature is obtained from the kinetic energy balance equation for the electron gas. The constraints of hydrostatic and radiative equilibrium are enforced throughout the model. A crude technique has been developed for the transfer of bound-bound radiation. The technique requires the definition of a mean absorption coefficient averaged over the line-absorption profile. Use of the technique permits the solution of the statistical equilibrium equations with no assumptions made concerning detailed balance for the bound-bound radiative processes. The source function is treated in microscopic detail. All atomic processes which contribute to the emission and absorption of radiation are considered. The kinetic energy balance equation for the electron gas is formulated in detail. All atomic processes by which kinetic energy is gained and lost by the electron gas are considered. Thomson scattering is included in the equation of transfer and radiation pressure effects are included in the hydrostatic equilibrium equation. The computational method contains three novel features which closely associate the algorithm with the real physical situation in a stellar atmosphere. First, a novel boundary condition is applied which is based on the requirement that deep in the atmosphere the local physical state of the material should asymptotically approach L.T.E. with the radiation field then locally determined as the Planck function at the local temperature. At a selected density in the atmosphere the material is assumed to be in L.T.E. at a certain selected temperature, and the radiation field is taken as characteristic of a black body at that temperature. This boundary condition differs from that used in other computation methods. In currently available methods the net flux of radiation escaping to interstellar space is used as a boundary condition for the determination of the physical structure throughout the atmosphere. The net outward flux is known before the computation begins but the physical conditions deep in the atmosphere are then unknown. The situation is reversed for the computational method described in this paper. The second novel feature is that the equilibrium physical state of the atmosphere is determined by a

relaxation technique. The third is that the radiative transfer problem is treated by the Monte Carlo technique. The iterative relaxation technique of obtaining the equilibrium physical state of the atmosphere is somewhat similar to the Λ-iteration technique used recently by LECAR (1965). His results showed that a purely iterative technique produces a solution which may well converge rather slowly. His work has shown that careful attention must be given to the rate at which convergence is being approached. In addition it must always be clearly demonstrated that the final apparently converged solution is stable. MIHALAS (1967b) has adopted a simple method of demonstrating that a solution has both stabilized and converged. His method is to begin by observing in which direction successive iterations are moving. The final apparently converged solution is forced beyond its stabilization point to see if it returns to its original stabilized value.

The theory on which the new computational method is based is described in Section 2. The method itself is described in Section 3. Subsection 3.A deals with the relaxation method for obtaining the equilibrium physical state of the atmosphere. Subsection 3.B deals with the Monte Carlo technique for transferring radiant energy throughout the atmosphere. Section 4 contains the results of a trial application of the method to the computation of a model atmosphere for a pure hydrogen early-type star. For this calculation the hydrogen atom was approximated by an idealized model containing five bound levels and the continuum. Section 5 discusses the solution with reference to its stability, accuracy, and convergence.

2. Theory

The equations describing the physical theory used in the model atmosphere computation have been formulated for the case of a pure hydrogen early-type star. Each volume element of the atmosphere is assumed to contain only electrons, protons, neutral hydrogen atoms, and photons. Specifically, both molecular hydrogen and negative hydrogen ions are assumed to be absent. The hydrogen atom is approximated by an idealized model containing five bound levels and the continuum. Although in principle any number of bound levels may be included in the atomic model for practical reasons the number was restricted to five. The theory is described below in considerable detail to clarify the subsequent discussion of the Monte Carlo transfer technique.

A. THE EQUATION OF RADIATIVE TRANSFER

If the atmosphere is assumed to be approximated by homogeneous plane parallel layers the equation of transfer may be written as

$$\left.\begin{aligned}\mu \frac{\mathrm{d}I_\lambda}{\mathrm{d}z}(z,\mu) = \frac{j_\lambda(z)}{4\pi} - K'_\lambda(z)\, I_\lambda(z,\mu) - \sigma_s(z)\, I_\lambda(z,\mu) \\ + \tfrac{3}{16}\sigma_s(z)\left[(3-\mu^2)\int_{-1}^{+1} I_\lambda(z,\mu')\,\mathrm{d}\mu' + (3\mu^2-1)\int_{-1}^{+1} I_\lambda(z,\mu')\,\mu'^2\,\mathrm{d}\mu'\right],\end{aligned}\right\} \tag{1}$$

where $\mu = \cos\theta$, where θ is the angle between the direction of the beam of light and the outward normal z to the surface of the star. The intensity of the radiation in direction μ at wavelength λ, in ergs $\mathrm{cm}^{-2}\ \mathrm{sec}^{-1}\ \text{Å}^{-1}$ steradian^{-1}, is given by $I_\lambda(z, \mu)$. The equation contains both thermal and scattering terms, since electron scattering can be an important source of opacity in early-type stars. The first term on the right-hand side of the equation, $j_\lambda(z)/4\pi$, gives the amount of radiant energy emitted spontaneously at wavelength λ, in ergs $\mathrm{cm}^{-3}\ \mathrm{sec}^{-1}\ \text{Å}^{-1}$ steradian^{-1}. The second term, $K'_\lambda(z) I_\lambda(z, \mu)$, gives the amount of energy absorbed from the beam, corrected for stimulated emission. The third term, $\sigma_s(z) I_\lambda(z, \mu)$, gives the loss of energy from the beam due to Thomson scattering. Finally, the fourth term takes account of Thomson scattering of radiant energy into the direction μ from all other directions μ' integrated over azimuth. Rather than assume an isotropic electron-scattering phase function the anisotropy of Thomson scattering has been included in the transfer equation. Choice of the Monte Carlo method for treating the radiative transfer problem enables an anisotropic phase function to be dealt with in the calculation just as easily and accurately as an isotropic phase function.

If the source function, $S_\lambda(z, \mu)$, is written as

$$S_\lambda(z, \mu) = \frac{1}{[K'_\lambda(z) + \sigma_s(z)]} \left\{ \frac{j_\lambda(z)}{4\pi} + \tfrac{3}{16}\sigma_s(z) \left[(3 - \mu^2) \int_{-1}^{+1} I_\lambda(z, \mu')\, \mathrm{d}\mu' + (3\mu^2 - 1) \int_{-1}^{+1} I_\lambda(z, \mu')\, \mu'^2\, \mathrm{d}\mu' \right] \right\} \tag{2}$$

the equation of transfer reduces to

$$\mu\, \mathrm{d}I_\lambda / \mathrm{d}\tau_\lambda(z, \mu) = I_\lambda(z, \mu) - S_\lambda(z, \mu), \tag{3}$$

where

$$\mathrm{d}\tau_\lambda = -\{K'_\lambda(z) + \sigma_s(z)\}\, \mathrm{d}z \tag{4}$$

and τ_λ is the optical depth at wavelength λ.

The linear scattering coefficient $\sigma_s(z)$ is given by

$$\sigma_s(z) = N_e(z)\, \sigma, \tag{5}$$

where σ is the Thomson scattering cross-section for an electron. N_e is the number density, in cm^{-3}, of free electrons.

If stimulated emission is treated as negative absorption in the manner outlined by HUMMER (1965) it may be readily shown that the linear absorption coefficient, $K'_\lambda(z)$, corrected for stimulated emission, is given by

$$K'_\lambda = K_\lambda - \frac{\lambda^5}{8\pi hc^2} j_\lambda, \tag{6}$$

where K_λ is the linear absorption coefficient, uncorrected for stimulated emission. If the quantity $j_\lambda/(4\pi K'_\lambda)$ is equal to $B_\lambda(T)$, the Planck function for temperature T

and wavelength λ, K'_λ is given by

$$K'_\lambda = \{1 - \exp[-hc/\lambda kT]\} K_\lambda , \tag{7}$$

where the symbols c, h, and k have their usual meanings.

The absorption coefficient K_λ may be written as

$$K_\lambda = K_{\lambda\mathrm{BF}} + K_{\lambda\mathrm{FF}} + K_{\lambda\mathrm{BB}} \tag{8}$$

for wavelengths where line absorption is present. The first of the three terms contributing to the absorption coefficient, $K_{\lambda\mathrm{BF}}$, is the linear bound-free opacity due to photo-ionization. The second term, $K_{\lambda\mathrm{FF}}$, is the linear free-free opacity. The third term, $K_{\lambda\mathrm{BB}}$, is the linear bound-bound opacity due to photo-excitation.

The corresponding spontaneous volume emission coefficient may be written as

$$j_\lambda = j_{\lambda\mathrm{FB}} + j_{\lambda\mathrm{FF}} + j_{\lambda\mathrm{BB}} . \tag{9}$$

The first term, $j_{\lambda\mathrm{FB}}$, is the volume emission for normal radiative recombination. The second term, $j_{\lambda\mathrm{FF}}$, is the volume emission for the free-free process. The third, $j_{\lambda\mathrm{BB}}$, is the spontaneous volume emission for the bound-bound transition.

The quantity $K_{\lambda\mathrm{BF}}$ may be written as

$$K_{\lambda\mathrm{BF}} = \sum_n N_n \alpha_n(\lambda) , \tag{10}$$

where $\alpha_n(\lambda)$ is the photo-ionization cross-section from bound level n for wavelength λ. N_n is the number density, in cm^{-3}, of atoms in level n. The summation is carried out over all levels n, subject to the condition that

$$hc/\lambda \geqslant I_n , \tag{11}$$

where I_n is the ionization energy from level n to the base of the continuum.

The quantity $K_{\lambda\mathrm{FF}}$ may be written as

$$K_{\lambda\mathrm{FF}} = N_i N_\mathrm{e} \alpha_{\mathrm{FF}}(\lambda, T_\mathrm{e}) , \tag{12}$$

where N_i is the number density of protons, N_e is the number density of free electrons, and $\alpha_{\mathrm{FF}}(\lambda, T_\mathrm{e})$ is a function of wavelength λ and electron temperature T_e, with units cm^5.

The quantity $K_{\lambda\mathrm{BB}}$ may be written as

$$K_{\lambda\mathrm{BB}} = \frac{N_{n'} B_{n'n} hc}{4\pi\lambda_0} \Psi_{n'n}(\Delta\lambda) , \tag{13}$$

where $N_{n'}$ is the number density of atoms in level n' capable of absorbing radiation and being excited to level n, $B_{n'n}$ is the Einstein probability of photoabsorption for the transition, λ_0 is the central wavelength of the line, and $\Psi_{n'n}(\Delta\lambda)$ is the line-absorption profile. The line absorption profile is normalized such that

$$\int_{-\infty}^{+\infty} \Psi_{n'n}(\Delta\lambda)\, \mathrm{d}(\Delta\lambda) = 1 . \tag{14}$$

The line-absorption profile is a convolution of Doppler and Stark broadening and is a function of n, n', N_i, N_e, T_e, and $\Delta\lambda$, where $\Delta\lambda=(\lambda-\lambda_0)$. The convolution is carried out by six point Gauss-Hermite quadrature.

The quantity $j_{\lambda FB}$ may be written as

$$j_{\lambda FB} = N_i N_e \sum_n \beta_n(\lambda, T_e), \tag{15}$$

where $\beta_n(\lambda, T_e)$ is a function of wavelength and temperature for each level n. The summation is carried out for all values of n such that

$$hc/\lambda \geqslant I_n. \tag{16}$$

The quantity $j_{\lambda FF}$ may be written as

$$j_{\lambda FF} = N_i N_e \beta_{FF}(\lambda, T_e), \tag{17}$$

where $\beta_{FF}(\lambda, T_e)$ is a function of wavelength λ and temperature T_e. Like $\beta_n(\lambda, T_e)$, the function $\beta_{FF}(\lambda, T_e)$ has units ergs cm^3 sec^{-1} Å^{-1}.

The quantity $j_{\lambda BB}$ may be written as

$$j_{\lambda BB} = N_n A_{nn'}(hc/\lambda_0)\, \Phi_{nn'}(\Delta\lambda), \tag{18}$$

where $A_{nn'}$ is the Einstein spontaneous transition probability, and $\Phi_{nn'}(\Delta\lambda)$ is the normalized line-emission profile. The assumption is made that

$$\Phi_{nn'}(\Delta\lambda) = \Psi_{n'n}(\Delta\lambda). \tag{19}$$

In addition the stimulated emission profile is assumed to be identical with the spontaneous emission and photoabsorption profiles.

B. THE ELECTRON-TEMPERATURE EQUATION

The electron temperature may be obtained by solving the local kinetic energy balance equation for the electron gas.

Kinetic energy is lost from the electron gas by four atomic processes;

(i) Free-free emission,

(ii) Normal radiative recombination to all bound levels j,

(iii) Electron collisional excitation, summed over all possible bound-bound transitions,

(iv) Electron collisional ionization, summed over all bound levels j.

Kinetic energy is gained by the electron gas by the following inverse processes;

(i) Free-free absorption,

(ii) Photo-ionization from all bound levels j,

(iii) Electron collisional de-excitation, summed over all possible bound-bound transitions,

(iv) Three-body electron collisional recombination, summed over all bound levels j.

The assumption is made that no energy is gained or lost by the electron gas when it scatters radiation. The electron-temperature equation may be written as

$$\left.\begin{aligned}\int_0^\infty j_{\lambda\mathrm{FF}}\,\mathrm{d}\lambda + N_i N_\mathrm{e}\sum_{j=1}^{5} L_{ij} + N_\mathrm{e}\sum_{j=1}^{4} N_j \sum_{k=j+1}^{5} Q_{jk}E_{jk} + N_\mathrm{e}\sum_{j=1}^{5} N_j Q_{ji}E_{ji} \\ = \int_0^\infty \frac{K_{\lambda\mathrm{FF}}}{K_\lambda}\, a_\lambda\,\mathrm{d}\lambda + \sum_{j=1}^{5} N_j M_{ji} + N_\mathrm{e}\sum_{k=2}^{5}\sum_{j=1}^{k-1} N_k Q_{kj}E_{jk} + N_\mathrm{e}^2 N_i \sum_{j=1}^{5} Q_{ij}E_{ji}\end{aligned}\right\} \tag{20}$$

The left-hand side of the equation gives the kinetic energy lost from the electron gas, in ergs $\mathrm{cm}^{-3}\ \mathrm{sec}^{-1}$. The right-hand side gives the kinetic energy gained. The quantity a_λ is equal to $4\pi K'_\lambda J_\lambda$, the net amount of energy absorbed at wavelength λ in ergs $\mathrm{cm}^{-3}\ \mathrm{sec}^{-1}\ \text{Å}^{-1}$. The intensity averaged over all solid angles, J_λ, is given by

$$J_\lambda = \tfrac{1}{2}\int_{-1}^{+1} I_\lambda(\mu)\,\mathrm{d}\mu\,. \tag{21}$$

In addition, the terms L_{ij} and M_{ji} are defined by

$$L_{ij} = \int_0^{\lambda_{\mathrm{LIMIT}\ j}} \beta_j(\lambda, T_\mathrm{e})\,\frac{\lambda}{hc}\,e_\lambda\,\mathrm{d}\lambda \tag{22}$$

and

$$M_{ji} = 4\pi \int_0^{\lambda_{\mathrm{LIMIT}\ j}} \frac{\alpha_j(\lambda)}{K_\lambda}\,\frac{\lambda}{hc}\,K'_\lambda J_\lambda e_\lambda\,\mathrm{d}\lambda\,, \tag{23}$$

where

$$e_\lambda = hc/\lambda - E_{ji} \tag{24}$$

and

$$\lambda_{\mathrm{LIMIT}\ j} = hc/E_{ji}\,. \tag{25}$$

Q_{jk} is the electron collisional rate, in $\mathrm{cm}^3\ \mathrm{sec}^{-1}$, for excitation from the lower bound level j to the upper bound level k, and Q_{kj} is the corresponding rate for the inverse process of de-excitation from level k to level j. Q_{ji} is the electron collisional ionization rate, in $\mathrm{cm}^3\ \mathrm{sec}^{-1}$, from level j to the base of the continuum i, and Q_{ij} is the corresponding rate for the inverse process of three-body collisional recombination. E_{jk} is the energy, in ergs, required to raise an atom from a lower level j to a higher level k. E_{ji} is the ionization energy from level j to the base of the continuum.

The kinetic energy balance equation has been formulated on the assumption that the electrons maintain a Maxwellian velocity distribution of characteristic temperature T_e. For this assumption to be valid it is essential that the relaxation time for elastic electron-electron collisions is much shorter than the mean time an electron remains in the continuum state. The relaxation time may be calculated from formulae given

by SPITZER (1962). For the electron densities and temperatures expected in stellar photospheres the relaxation time is always orders of magnitude shorter than the mean lifetime of a free electron.

C. THE STATISTICAL EQUILIBRIUM EQUATIONS

The atomic and ionic level populations in any volume element of the atmosphere are obtained by solving the set of statistical equilibrium equations for each atom. Each equation of a set gives the rates at which atoms are entering and leaving a given energy state. In the steady state the rates of entry to and exit from each level are equal. For a hydrogen atomic model, with five bound levels and the continuum, the statistical equilibrium equation for each bound level j may be written as

$$\sum_{\substack{n=1 \\ n \neq j}}^{5} N_n U_{nj} + N_i U_{6j} - N_j U_{jj} = 0 . \tag{26}$$

For the continuum i the corresponding equation is

$$\sum_{n=1}^{5} N_n U_{n6} - N_i U_{66} = 0 . \tag{27}$$

The atomic level populations are subject to the condition that

$$\sum_{n=1}^{5} N_n + N_i = N_{\text{TOTAL}} , \tag{28}$$

where

$$N_{\text{TOTAL}} = \rho / m_{\text{H}} , \tag{29}$$

where ρ is the density in grms cm^{-3}, and m_{H} is the mass of the hydrogen atom in grms.

The following atomic processes must be considered in the evaluation of the U_{jk} terms;

(a) Spontaneous bound-bound emission.
(b) Induced bound-bound emission.
(c) Photoexcitation.
(d) Photo-ionization.
(e) Normal radiative recombination.
(f) Induced radiative recombination.
(g) Electron collisional excitation.
(h) Electron collisional de-excitation.
(i) Electron collisional ionization.
(j) Electron collisional recombination.

Induced, or stimulated, emission is treated as negative absorption. Detailed balance is not assumed for the bound-bound radiative transitions.

For $n' < n$, $n \leqslant 5$, $n \neq n'$

$$U_{n'n} = \frac{4\pi}{N_{n'} E_{n'n}} \int_{-\infty}^{+\infty} \frac{K_{\lambda BB}}{K_\lambda} K'_\lambda J_\lambda \, \mathrm{d}(\Delta\lambda) + N_e Q_{n'n} \tag{30}$$

$$U_{nn'} = A_{nn'} + N_e Q_{nn'} . \tag{31}$$

For $j \leqslant 5$,

$$\left.\begin{aligned} U_{jj} = \sum_{\substack{k=1 \\ j>1}}^{j-1} A_{jk} + \frac{4\pi}{N_j} \sum_{k=j+1}^{5} \frac{1}{E_{jk}} \int_{-\infty}^{+\infty} \frac{K_{\lambda BB}}{K_\lambda} K'_\lambda J_\lambda \, \mathrm{d}(\Delta\lambda) \\ + \frac{4\pi}{hc} \int_0^{\lambda_{\mathrm{LIMIT}\ j}} \frac{\alpha_j(\lambda)}{K_\lambda} K'_\lambda J_\lambda \lambda \, \mathrm{d}\lambda + N_e \sum_{\substack{k=1 \\ j \neq k}}^{5} Q_{jk} + N_e Q_{ji} \end{aligned}\right\} \tag{32}$$

For $n = 6 = i$

$$U_{nn} = \frac{N_e}{hc} \sum_{n'=1}^{5} \int_0^{\lambda_{\mathrm{LIMIT}\ n'}} \beta_{n'}(\lambda, T_e) \, \lambda \, \mathrm{d}\lambda + N_e^2 \sum_{n'=1}^{5} Q_{nn'} . \tag{33}$$

For $n = 6 = i$, $n' < n$

$$U_{nn'} = \frac{N_e}{hc} \int_0^{\lambda_{\mathrm{LIMIT}\ n'}} \beta_{n'}(\lambda, T_e) \, \lambda \, \mathrm{d}\lambda + N_e Q_{nn'} . \tag{34}$$

D. THE EQUATION OF HYDROSTATIC EQUILIBRIUM

The equation of hydrostatic equilibrium is given by

$$\frac{\mathrm{d}P(z)}{\mathrm{d}z} = -\, g(z)\, \rho(z), \tag{35}$$

where $P(z)$ is the total pressure in dynes cm^{-2}, $g(z)$ is the surface gravity in $\mathrm{cm\ sec}^{-2}$, and $\rho(z)$ is the density in grms cm^{-3}. The quantity $\mathrm{d}P(z)/\mathrm{d}z$ is the sum of two terms, a gas-pressure term $\mathrm{d}P_g/\mathrm{d}z$ and a radiation pressure term $\mathrm{d}P_r/\mathrm{d}z$. The radiation-pressure term may be written as

$$\frac{\mathrm{d}P_r(z)}{\mathrm{d}z} = \frac{\pi}{c} \int_0^{\infty} \left(K'_\lambda(z) + \sigma_s(z)\right) F_\lambda(z) \, \mathrm{d}\lambda, \tag{36}$$

where

$$F_\lambda(z) = 2 \int_{-1}^{+1} I_\lambda(z, \mu) \, \mu \, \mathrm{d}\mu . \tag{37}$$

The quantity $\pi F_\lambda(z)$ is the net outward flux of radiation of wavelength λ at the position z in the atmosphere.

E. THE EQUATION OF RADIATIVE EQUILIBRIUM

The equation of radiative equilibrium is given by

$$\int_0^\infty j_\lambda(z)\,\mathrm{d}\lambda = 4\pi \int_0^\infty K'_\lambda(z)\,J_\lambda(z)\,\mathrm{d}\lambda \tag{38}$$

F. SOURCES OF ATOMIC DATA

For the hydrogen atom the Einstein probability coefficients $A_{nn'}$, $B_{nn'}$, and $B_{n'n}$, were obtained from WIESE *et al.* (1966). Bound-free photo-ionization cross-sections were computed for each level of the hydrogen atom as a function of wavelength from formulae given by MENZEL and PEKERIS (1935). For the inverse free-bound process, radiative recapture cross-sections and recombination rates were computed from the photo-ionization cross-sections by using the Milne relation. Free-free absorption and emission data for each wavelength, temperature, and electron density, were computed from formulae given by CILLIÉ (1932). To save computer time a simplified method of computing Stark broadening as a function of principal quantum number, electron density and temperature, was required. The approximate method developed by GRIEM (1960) was used. Electron collisional excitation and de-excitation rates were computed from formulae given by ALLEN (1963). De-excitation rates were obtained by the principle of detailed balance. Electron collisional ionization rates were computed from formulae given by GRYZINSKI (1964). Rates for the inverse process of three-body recombination were computed by the principle of detailed balance. Of all the atomic data used in the model atmosphere computation the electron collisional excitation rates and de-excitation rates are by far the most uncertain. Typically, errors of up to a factor of 2 or so may be expected in their absolute values. Unfortunately significantly better collisional cross-section data, on which the rates could be based, do not yet exist.

3. Computational Method

A. THE RELAXATION PROCESS

The atmosphere is approximated by a model containing a number of plane parallel zones. The physical conditions are assumed to be uniform throughout each zone. The zone boundaries are determined from the equation of hydrostatic equilibrium. The pressure ratio, p_i/p_{i+1}, between the boundaries i and $i+1$ of a given zone i normally may be taken as given by

$$\log_{10}(p_i/p_{i+1}) = 0.2\,. \tag{39}$$

The choice of 0.2 for the right-hand side of the equation is somewhat arbitrary. It represents a compromise. For practical reasons a fairly small number of zones must be used, but the entire atmosphere must still be adequately covered. Practical considerations restrict the number of zones to about 20. A further consideration in determining the zone boundaries is that each zone must not be so wide that the

assumption of its homogeneity in density and temperature becomes untenable. The density throughout each zone is obtained from the linear distance between the boundaries and from a knowledge of the mass of material contained in the zone.

The essential feature of the relaxation technique is the imposition of an initial non-equilibrium physical condition on every part of the atmosphere. The atmosphere is then permitted to go through a controlled relaxation until it reaches the steady equilibrium state. Instead of starting the iteration from an L.T.E. radiative equilibrium solution – an initial condition used in the Λ-iteration method – the initial physical state of the atmosphere is chosen to be *very far from* equilibrium. The objective in so doing is to permit a rapid relaxation *towards* equilibrium particularly during the first few iterations of the atmosphere. The relaxation is begun by arbitrarily assuming the atmosphere is initially isothermal at the lower-base boundary temperature and in L.T.E. throughout. In its initial state the atmosphere is very far from radiative equilibrium. The outer layers of the atmosphere will cool from their initial high-temperature state during successive iterations. The cooling of any zone of the atmosphere indicates a local imbalance between photo-ionization and radiative recombination. The imbalance is such that the number of photo-ionizations is less than the number of radiative recombinations. As the zone cools substantial recombination from the continuum will occur. The atomic level populations will increase and move towards their equilibrium values. The relaxation proceeds until every part of the atmosphere reaches equilibrium.

The lower-base boundary of the atmosphere is assumed to be a black-body surface characterized by a density ρ_0 and a temperature T_0. A flux of black-body radiation of characteristic temperature T_0 is fed into the atmosphere across the lower boundary. Radiation flowing downward from higher regions of the atmosphere which strikes the lower boundary is totally absorbed. However, the adopted boundary temperature remains fixed throughout the computation of the model atmosphere.

Hydrostatic equilibrium is assumed and the atomic and ionic level populations of each zone are set initially at their L.T.E. values for the local temperature. Initially the atmosphere is assumed to contain no radiation. It is then released from its stretched condition, and the radiation spontaneously emitted per second from every part of the atmosphere is transferred by Monte Carlo source particles as described in the following section. During the transfer of the radiation the physical state of the atmosphere is arbitrarily held constant. No attempt is made to follow the relaxation of the physical parameters with time. After the transfer is completed, and all the radiant energy carried by the source particles has either been reabsorbed or escaped into interstellar space, the energy absorbed in each zone is used to determine the new physical state of the atmosphere. The atomic and ionic level populations, the electron densities and temperatures, and the departures of the level populations from their L.T.E. values are determined for all zones. Escape of radiation from the outermost zones causes them to cool, contract, and become denser. The entire atmosphere becomes much less distended. The condition of radiative equilibrium is applied and the solution is iterated until convergence is reached.

If for each zone $K'_\lambda J_\lambda$ is known as a function of wavelength, from the Monte Carlo transfer technique, the terms in the equations of statistical equilibrium and in the electron-temperature equation can be evaluated. The atomic and ionic level populations and the electron temperature can be determined by an iterative technique. The determination of the absorption coefficient at any wavelength for use in the Monte Carlo transfer requires a knowledge of the temperature, density and atomic level populations, which must be obtained either from a previous iteration of the atmosphere or by assumption.

At the end of each iteration of the atmosphere the physical state of each zone is determined by a relaxation technique. To determine the range in which the electron temperature must lie, a sequence of trial temperatures are used in the solution of the statistical equilibrium equations and in balancing the electron-temperature equation. For each temperature the equations of statistical equilibrium are solved first and the new populations are used in testing the balance of the electron-temperature equation. If the energy gained by the electron gas is greater than the energy lost the adopted temperature is too low. Vice versa the temperature is too high. The range in which the electron temperature must lie is repeatedly halved following each test of a trial temperature. If the correct temperature is expected to lie between 0 and 10^6 K, for example, it may be obtained to an accuracy of 1 K after only 18 trial solutions ($2^{18} \approx 10^6$).

An iterative technique must be used to solve the statistical equilibrium equations since the equations are non-linear in the electron density, N_e. If N_e is known, the equations become linear. The iteration starts with N_e set at zero. The statistical equilibrium equations are then solved, and N_e is reset to equal the number density of ions. The iteration is continued until N_e and the atomic and ionic level populations converge.

Some difficulty was encountered in solving the linearized statistical equilibrium equations, particularly when the number of ions was very much greater than the sum of the populations of the atoms in the bound levels. The Gauss-Jordan elimination method was found to produce non-physical results due to the ill-conditioned nature of the equations. In particular negative values for the atomic level populations could occur. To overcome these difficulties an alternative method of solution was developed.

We have the condition

$$\sum_{j=1}^{5} N_j + N_i = N_{\text{TOTAL}} . \tag{40}$$

In the steady state

$$N_j U_{j6} = N_i U_{6j} , \quad 1 \leqslant j \leqslant 5 , \tag{41}$$

so that

$$\frac{N_j}{N_i} = \frac{U_{6j}}{U_{j6}} = R_j , \quad 1 \leqslant j \leqslant 5 , \quad \text{and} \quad R_6 = 1.0 . \tag{42}$$

The value of N_i is given by

$$N_i = N_{\text{TOTAL}} / \sum_{j=1}^{6} R_j . \tag{43}$$

The values of N_j, $1 \leqslant j \leqslant 5$, may be obtained from

$$N_j = N_i R_j . \tag{44}$$

The total number of neutral atoms, $N_{\text{Total Neutral}}$, may be obtained from

$$N_{\text{Total Neutral}} = \sum_{j=1}^{5} N_j . \tag{45}$$

Further values of N_k, $1 \leqslant k \leqslant 5$, may be obtained from the following considerations. In the steady state

$$N_j U_{jk} = N_k U_{kj} , \quad \text{for } j \neq k,\ 1 \leqslant j \leqslant 5,\ 1 \leqslant k \leqslant 5 , \tag{46}$$

so that

$$\frac{N_j}{N_k} = \frac{U_{kj}}{U_{jk}} = R_j , \quad \text{for } j \neq k,\ 1 \leqslant j \leqslant 5,\ 1 \leqslant k \leqslant 5 , \quad \text{and}$$

$$R_j = 1.0 , \quad \text{for } j = k . \tag{47}$$

It follows that

$$N_k = N_{\text{Total Neutral}} / \sum_{j=1}^{6} R_j . \tag{48}$$

In addition

$$N_j = N_k R_j , \quad \text{for } j \neq k,\ 1 \leqslant j \leqslant 5,\ 1 \leqslant k \leqslant 5 . \tag{49}$$

The average value of N_j, $1 \leqslant j \leqslant 5$, is obtained finally. A normalization check of this value is made by multiplying it by

$$N_{\text{Total Neutral}} / \sum_{j=1}^{5} N_j ,$$

where the values of N_j used in the summation are the average values before normalization.

The techniques for solving the statistical equilibrium equations and the electron-temperature equation were tested by using them to determine the physical state of a volume element of the stellar atmosphere, of density ρ, illuminated by an isotropic black-body radiation field of characteristic temperature T. In these tests no assumptions were made concerning detailed balance for the bound-bound radiative transitions. Several widely different combinations of ρ and T were used as test cases, e.g. $T = 50000\,\text{K}$, $\rho = 5 \times 10^{-8}$ grms cm^{-3} and $T = 10000\,\text{K}$, $\rho = 10^{-11}$ grms cm^{-3}. For these ranges in density and temperature it was found that, provided the radiation field was known, the most useful starting-condition for the solution of the physical state of the gas was to assume that initially all atoms are ionized. The solutions of the statistical equilibrium equations, and the electron temperature equation, were iterated until the electron-number density and the atomic and ionic level populations had converged to an accuracy of 0.5% and the electron temperature had converged to an accuracy of 1%. Progressive recombination from the continuum appears to occur rapidly during successive iterations. No more than three iterations were ever required to obtain the above level of accuracy. In each of the test cases which were considered

the electron-number density and the atomic and ionic level populations rapidly converged to the appropriate L.T.E. values for a temperature T and density ρ. The electron temperature converged to the radiation temperature, T. Of course, the solutions could readily have been iterated further to attain greater accuracy. However, the above accuracy was adopted for the exploratory calculations with the relaxation technique which are reported below. It may be remarked that only those departures from L.T.E. in the atomic level populations which are greater than 0.5% will then be detectable. In particular, such small departures reported by MIHALAS (1967b, c) will not be detected unless the accuracy of the solution is increased considerably.

B. MONTE CARLO RADIATIVE TRANSFER

Recently FLECK (1963) has demonstrated the Monte Carlo technique for solving non-linear radiation transport problems. The simplicity of the method, its inherent stability, and the ease with which anisotropic scattering phase functions may be treated, make it an attractive technique for handling radiative transfer in stellar atmospheres. It may be remarked, however, that the price paid for simplicity is the necessity of using a considerable amount of high-speed computer time, so that enough Monte Carlo events occur to obtain good statistical accuracy in the final results.

The essence of the Monte Carlo technique is that the radiant energy emitted per second from every part of the atmosphere at each wavelength is carried by a very large number of source particles which have some of the properties of photons. A separate species of source particle is used to transfer radiation of each wavelength. In their migration through the atmosphere these source particles interact with the stellar material with the absorption of part of their energy and scattering of the remainder. The amount of radiant energy associated with a source particle at any point in its migration is given by its 'weight', which steadily decreases with each interaction with matter. A tally is kept of the amount of energy deposited in each zone by each species of source particle to determine $K'_\lambda J_\lambda$ as a function of wavelength. If $K'_\lambda J_\lambda$ is known as a function of wavelength the electron-temperature equation and the equations of statistical equilibrium can be solved.

The evaluation of the terms in the electron-temperature equation and in the statistical equilibrium equations requires the integration of the bound-free and free-free absorption over the continuum wavelengths. The quantity $K'_\lambda J_\lambda$ is discontinuous at the Lyman, Balmer, Paschen, Brackett, and Pfund series limits. The amount of radiant energy excluded from the calculation by truncating the wavelength range at 10 and 50000 Å is negligible. By using six-point Gaussian quadrature for each of the 6 segments radiant energy need be transferred at no more than 36 individual continuum wavelength points to determine the bound-free and free-free absorption in each zone.

A similar procedure for obtaining the bound-bound absorption integrals for each zone, by transferring radiation at a very limited number of Gaussian wavelength points within each line, cannot be used in the case of an inhomogeneous atmosphere. Changes in density and temperature throughout the atmosphere severely affect the

absorption and emission profiles for each bound-bound transition. Temperature differences alter the width of the Doppler core, while density differences alter the shape of the Stark wings. Wavelength points chosen deep in the atmosphere will be unsuitable for the more tenuous outer regions where the profile is much narrower.

For the transfer of bound-bound radiation all the radiant energy, integrated over a wavelength band centered on and containing the line associated with the particular transition, is carried throughout the atmosphere in one species of source particle. Background continuum radiation arising from free-bound and free-free emission is also transferred in the same species of source particle. To follow the transfer of these source particles from one part of the atmosphere to another it is necessary to define an appropriate mean absorption coefficient for the band. Before discussing how such a mean absorption coefficient may be defined it should be pointed out that such an approach to the transfer of bound-bound radiation is very crude indeed. The crudity of the treatment is unfortunately dictated by practical considerations for the problem to become computationally tractable.

The calculation of a mean absorption coefficient for the band is based on the following considerations. Consider the transmission of radiation in a wavelength band of width $2\,\Delta\lambda_{\text{LIMIT}}$ through a homogeneous slab of atmospheric material of thickness x. The radiation is assumed to be striking the slab at normal incidence. The band contains radiation which originated in the free-free and free-bound emission processes as well as radiation which originated in bound-bound radiative decays. For simplicity Thomson scattering is not included in the determination of the transmission of the radiation in the band. Its inclusion would not affect the subsequent definition of the mean linear opacity for bound-bound absorption for the band. The transmission through the slab may be written

$$\int_{\text{BAND}} [I_c(\lambda) - I_l(\lambda)] \exp[-(K_c'(\lambda) + K_l'(\lambda))\, x]\, \mathrm{d}\lambda\,,$$

where $I_c(\lambda)$ is the intensity of the background continuum radiation of wavelength λ incident on the slab, $I_l(\lambda)$ is the intensity of the bound-bound radiation of wavelength λ incident on the slab, $K_c'(\lambda)$ is the continuum linear opacity, corrected for stimulated emission, which contains contributions from free-free and bound-free photoabsorption, $K_l'(\lambda)$ is the bound-bound linear opacity, corrected for stimulated emission.

A mean linear opacity, $\bar{K}'$, corrected for stimulated emission, may be defined for the band such that the total transmission integrated over the band remains the same as before. In that case we have

$$\left.\begin{aligned} \exp[-\bar{K}'x] \int_{\text{BAND}} [I_c(\lambda) + I_l(\lambda)]\, \mathrm{d}\lambda \\ = \int_{\text{BAND}} [I_c(\lambda) + I_l(\lambda)] \exp[-(K_c'(\lambda) + K_l'(\lambda))\, x]\, \mathrm{d}\lambda\,. \end{aligned}\right\} \tag{50}$$

If we write

$$\bar{\tau} = \bar{K}' x \tag{51}$$

and

$$\tau_c(\lambda) = K_c'(\lambda)\, x \tag{52}$$

with

$$\tau_l(\lambda) = K_l'(\lambda)\, x\,, \tag{53}$$

we have

$$\left.\begin{aligned} &\exp(-\bar{\tau}) \int_{\text{BAND}} [I_c(\lambda) + I_l(\lambda)]\, \mathrm{d}\lambda \\ &\qquad = \int_{\text{BAND}} [I_c(\lambda) + I_l(\lambda)] \exp[-(\tau_c(\lambda) + \tau_l(\lambda))]\, \mathrm{d}\lambda\,. \end{aligned}\right\} \tag{54}$$

If the approximation is made that $K_c'(\lambda)$ is independent of wavelength over the band considered we have

$$\left.\begin{aligned} &\exp(-\bar{\tau}) \int_{\text{BAND}} [I_c(\lambda) + I_l(\lambda)]\, \mathrm{d}\lambda \\ &\qquad = \exp[-\tau_c] \int_{\text{BAND}} [I_c(\lambda) + I_l(\lambda)] \exp[-\tau_l(\lambda)]\, \mathrm{d}\lambda\,. \end{aligned}\right\} \tag{55}$$

The approximation is also made that $I_c(\lambda)$ is independent of wavelength over the band. For convenience the quantity I_{L} is defined such that

$$\int_{-\Delta\lambda_{\text{LIMIT}}}^{+\Delta\lambda_{\text{LIMIT}}} I_l(\lambda)\, \mathrm{d}\lambda = I_{\text{L}}\,. \tag{56}$$

We have then

$$\left.\begin{aligned} &\exp[-\bar{\tau}]\, \{2I_c\, \Delta\lambda_{\text{LIMIT}} + I_{\text{L}}\} \\ &\qquad = \exp[-\tau_c] \int_{-\Delta\lambda_{\text{LIMIT}}}^{+\Delta\lambda_{\text{LIMIT}}} [I_c + I_l(\lambda)] \exp[-\tau_l(\lambda)]\, \mathrm{d}\lambda\,. \end{aligned}\right\} \tag{57}$$

If $\bar{\tau}_{\text{BB}}$ is defined by

$$\bar{\tau}_{\text{BB}} = \bar{\tau} - \tau_c \tag{58}$$

we have

$$\left.\exp[-\bar{\tau}_{\text{BB}}]\, \{2I_c\, \Delta\lambda_{\text{LIMIT}} + I_{\text{L}}\} = \int_{-\Delta\lambda_{\text{LIMIT}}}^{+\Delta\lambda_{\text{LIMIT}}} [I_c + I_l(\lambda)] \exp[-\tau_l(\lambda)]\, \mathrm{d}\lambda\,.\right\} \tag{59}$$

The exponential terms on both sides of the equation may be expanded into their corresponding series forms. If terms of second and higher order in $\bar{\tau}_{\text{BB}}$ and $\tau_l(\lambda)$ are neglected in the expansion we have

$$[2I_c\, \Delta\lambda_{\text{LIMIT}} + I_{\text{L}}]\, \bar{\tau}_{\text{BB}} = \int_{-\Delta\lambda_{\text{LIMIT}}}^{+\Delta\lambda_{\text{LIMIT}}} [I_c + I_l(\lambda)]\, \tau_l(\lambda)\, \mathrm{d}\lambda\,. \tag{60}$$

Dividing Equation (60) through by x we have the definition of $\bar{K}'_{\mathrm{BB}}$, which is

$$\bar{K}'_{\mathrm{BB}} = \frac{\int_{-\Delta\lambda_{\mathrm{LIMIT}}}^{+\Delta\lambda_{\mathrm{LIMIT}}} [I_c + I_l(\lambda)]\, K'_l(\lambda)\, \mathrm{d}\lambda}{[I_{\mathrm{L}} + 2I_c\, \Delta\lambda_{\mathrm{LIMIT}}]}. \tag{61}$$

We know that

$$K_{\lambda\mathrm{BB}} = \frac{N_{n'} B_{n'n}}{[N_{n'} B_{n'n} - N_n B_{nn'}]} K'_{\lambda\mathrm{BB}}, \tag{62}$$

where N_n, $N_{n'}$ are the number densities for atomic levels n and n' respectively. It follows that

$$\bar{K}_{\mathrm{BB}} = \frac{N_{n'} B_{n'n}}{[N_{n'} B_{n'n} - N_n B_{nn'}]} \bar{K}'_{\mathrm{BB}}, \tag{63}$$

where $\bar{K}_{\mathrm{BB}}$ is the mean linear opacity for bound-bound absorption for the band, uncorrected for stimulated emission.

For an inhomogeneous atmosphere, in which the band radiation is transferred by Monte Carlo source particles, the quantity $\bar{K}_{\mathrm{BB}}$ relevant to the transfer of any particular particle is a function of the zone i of origin of the particle and of the zone j in which interaction with matter occurs. The corresponding mean linear opacity, $\bar{K}_{ij}$, is defined by

$$\bar{K}_{ij} = \bar{K}_{\mathrm{BB}ij} + K_{\lambda\mathrm{BF}} + K_{\lambda\mathrm{FF}}, \tag{64}$$

where $K_{\lambda\mathrm{BF}}$ and $K_{\lambda\mathrm{FF}}$ are, respectively, the bound-free and free-free linear absorption coefficients for zone j and wavelength λ_0. The mean bound-bound opacity $\bar{K}_{\mathrm{BB}ij}$ may be obtained from

$$\bar{K}_{\mathrm{BB}ij} = \frac{\int_{-\Delta\lambda_{\mathrm{LIMIT}}}^{+\Delta\lambda_{\mathrm{LIMIT}}} j_\lambda K_{\lambda\mathrm{BB}}\, \mathrm{d}\lambda}{\int_{-\Delta\lambda_{\mathrm{LIMIT}}}^{+\Delta\lambda_{\mathrm{LIMIT}}} j_\lambda\, \mathrm{d}\lambda}, \tag{65}$$

where the emission coefficient, j_λ, refers to zone i, and $K_{\lambda\mathrm{BB}}$ refers to zone j.

The corresponding mean linear opacity for the band, corrected for stimulated emission, is given by

$$\bar{K}'_{ij} = \bar{K}'_{\mathrm{BB}ij} + K'_{\lambda\mathrm{BF}} + K'_{\lambda\mathrm{FF}}, \tag{66}$$

where

$$(K'_{\lambda\mathrm{BF}} + K'_{\lambda\mathrm{FF}}) = (K_{\lambda\mathrm{BF}} + K_{\lambda\mathrm{FF}}) - \frac{\lambda_0^5}{8\pi hc^2} (j_{\lambda\mathrm{FB}} + j_{\lambda\mathrm{FF}}) \tag{67}$$

The quantities $K_{\lambda\mathrm{BF}}$, $K_{\lambda\mathrm{FF}}$, $j_{\lambda\mathrm{FB}}$, and $j_{\lambda\mathrm{FF}}$, refer to zone j.

The band width, $2\Delta\lambda_{\mathrm{LIMIT}}$, is obtained by choosing $\Delta\lambda_{\mathrm{LIMIT}}$ such that

$$\Phi_i(\Delta\lambda_{\mathrm{LIMIT}}) = 0.01\Phi_i(0), \tag{68}$$

where $\Phi_i(\Delta\lambda)$ is the normalized emission profile for the bound-bound transition for zone i. If zone i is the lower base boundary, then $\Phi_i(\Delta\lambda)$ is independent of wavelength. In that case the value of $\Delta\lambda_{\text{LIMIT}}$ is taken as that appropriate for the zone immediately above the lower boundary. The integrals used to determine $\bar{K}_{\text{BB}i,j}$ are symmetrical about $\Delta\lambda=0$. Six-point Gaussian quadrature is used for the integration between 0 and $\Delta\lambda_{\text{LIMIT}}$.

A question immediately arises concerning the validity of the choice of a mean opacity for the transfer of bound-bound radiation. In particular, in what sense will the transmission through any linear thickness, x, of gas be distorted by such a choice? That question may be answered qualitatively by examining certain simplified cases.

The idealized case of the transmission of radiation in a Doppler-broadened emission line through a gaseous medium composed of atoms with only two energy levels has been considered briefly by IVANOV and SHCHERBAKOV (1965). The simplest case they considered was where the absorption profile is Doppler shaped with the same central wavelength and width as that of the incident emission line. Their results show that the transmission, integrated over the line, decreases monotonically with increasing optical thickness at the central wavelength. As the optical thickness gradually increases from zero the rate at which the transmission decreases is very rapid at first, becoming slower as the thickness becomes large and transmission in the wings of the line increases rapidly in importance relative to transmission near the line center. Suppose now that $\bar{K}'_{\text{BB}}$ is determined for this idealized case in the manner outlined above. From the results obtained by Ivanov and Shcherbakov it is not difficult to show that the *correct* integrated transmission will always be greater than $\exp(-\bar{K}'_{\text{BB}}x)$ for all x greater than zero. The ratio of the correct to the distorted transmission $\exp(-\bar{K}'_{\text{BB}}x)$, approaches unity as x tends to zero, and becomes progressively larger as x increases. As we shall see shortly, the curve of transmission vs. optical thickness is used in choosing the distances travelled between collisions by the bound-bound Monte Carlo source particles. To ease the computational problem, the curve of $\exp(-\bar{K}'_{\text{BB}}x)$ vs. x is used in place of the *correct* transmission curve for choosing these distances. Consequently the tendency will always be to underestimate the distances travelled between collisions by each of these source particles. The net effect for the transfer of a large number of source particles will be to underestimate the transmission of the bound-bound radiation, particularly through large optical thicknesses.

Suppose now that the Doppler width of the incident line is greater than that of the absorption profile. Such a case is analogous to the transfer of a flux of bound-bound radiation from a high-temperature region of a stellar atmosphere through lower-temperature regions into interstellar space. The integrated transmission will be greater than in the case where the Doppler widths are equal, because of the increased relative importance of transmission in the wings of the line. Again, the effect of using the $\exp(-\bar{K}'_{\text{BB}}x)$ transmission curve in the transfer of the bound-bound source particles will be to underestimate the integrated transmission.

It follows that the escape of bound-bound source particles from the atmosphere

will be inhibited by our adopted method of treating their transfer through the gas. Consequently, departures from detailed balance for the bound-bound radiative processes, arising from the escape of bound-bound radiation from the atmosphere, and the resultant departures from L.T.E. in the atomic level populations, will be underestimated.

Source particles originating from the lower-base black-body boundary are not emitted isotropically into the upward hemisphere. The number of photons crossing this surface from below in any given direction is weighted by μ_0, the cosine of the angle which this direction makes with the z-direction. The quantity μ_0 is obtained from the relation

$$\mu_0 = \text{Max}(r_1, r_2), \tag{69}$$

where r_1 and r_2 are two uniform random numbers between 0 and 1. μ_0 is set equal to the larger of the pair. The initial weight, ω_0, of each continuum source particle of each species emitted from the lower-base boundary is given by

$$\omega_0 = \frac{\pi B_\lambda(T_0)}{n_B}, \tag{70}$$

where $B_\lambda(T_0)$ is the Planck function, in ergs cm^{-2} sec^{-1} Å^{-1} steradian^{-1}, for wavelength λ and temperature T_0. n_B is the number of source particles of that particular species which originate in the lower base. The corresponding value of ω_0 for a bound-bound source particle is given by

$$\omega_0 = \frac{2\pi B_{\lambda_0}(T_0)\, \Delta\lambda_{\text{LIMIT}}}{n_B}, \tag{71}$$

where $B_\lambda(T_0)$ is assumed not to vary over the wavelength band. $\Delta\lambda_{\text{LIMIT}}$ is obtained from

$$\Phi(\Delta\lambda_{\text{LIMIT}}) = 0.01\Phi(0), \tag{72}$$

where $\Phi(\Delta\lambda)$ is the emission profile for the zone immediately above the lower base.

Source particles originating from each of the zones are emitted isotropically, and uniformly at random in z, throughout the thickness of the zone. The direction of emission, μ_0, is obtained from the relation

$$\mu_0 = 2r - 1, \tag{73}$$

where r is a uniform random number between 0 and 1. The initial weight, ω_0, of each continuum source particle of each species emitted from a zone of thickness Δz is given by

$$\omega_0 = \frac{j_\lambda\, \Delta z}{n_z}. \tag{74}$$

n_z is the number of source particles of that particular species which originate in the zone. The corresponding value of ω_0 for a bound-bound source particle is given by

$$\omega_0 = \frac{\Delta z}{n_z} \int_{-\Delta\lambda_{\text{LIMIT}}}^{\Delta\lambda_{\text{LIMIT}}} j_\lambda \, \mathrm{d}(\Delta\lambda). \tag{75}$$

In this case $\Delta\lambda_{\text{LIMIT}}$ is obtained from

$$\Phi(\Delta\lambda_{\text{LIMIT}}) = 0.01\Phi(0), \tag{76}$$

where $\Phi(\Delta\lambda)$ is the emission profile for that zone.

For any given source particle the distance, d_B, it must travel to reach the boundary of its current zone may be computed readily from a knowledge of its current location and direction of motion. The distance, d_{col}, travelled before a photon-matter interaction occurs may be obtained from

$$d_{\text{col}} = \eta \, |\log_e r| \, , \tag{77}$$

where r is a uniform random number between 0 and 1. η is the current mean free path of the source particle and may be written as

$$\eta = [K'_\lambda + \sigma_s]^{-1} \tag{78}$$

for the transfer of continuum radiation, and as

$$\eta = [\bar{K}'_{ij} + \sigma_s]^{-1} \tag{79}$$

for the transfer of bound-bound radiation.

If $d_B > d_{\text{col}}$ the source particle suffers an interaction in its current zone. If ω is the 'weight' of the source particle before an interaction, the weight following interaction is

$$\left\{\frac{\sigma_s}{K_\lambda + \sigma_s}\right\} \omega$$

if the source particle is transferring continuum radiation, and

$$\left\{\frac{\sigma_s}{\bar{K}_{ij} + \sigma_s}\right\} \omega$$

if it is transferring both bound-bound and background continuum radiation. The quantity

$$\left\{\frac{\sigma_s}{K_\lambda + \sigma_s}\right\}, \quad \text{or} \quad \left\{\frac{\sigma_s}{\bar{K}_{ij} + \sigma_s}\right\}$$

is the fraction of the continuum or bound-bound energy, respectively, associated with the source particle, which is scattered by the free electrons at the point of interaction. The quantity

$$\left\{\frac{K_\lambda}{K_\lambda + \sigma_s}\right\}, \quad \text{or} \quad \left\{\frac{\bar{K}_{ij}}{\bar{K}_{ij} + \sigma_s}\right\}$$

is the corresponding fraction of the energy absorbed by the material at the point of interaction. In the case of the absorption of bound-bound and background continuum radiation only the fraction

$$\bar{K}_{\mathrm{BB}ij}/\bar{K}_{ij}$$

is absorbed in the bound-bound transition itself, and included in the tally of energy absorbed for the particular transition.

If $d_B < d_{\mathrm{col}}$, a zone boundary is crossed. The value of d'_B, the distance the particle must travel to reach the other boundary of the new zone, is readily computed. The value of d'_{col} for the new zone is obtained from

$$d'_{\mathrm{col}} = (\eta'/\eta)(d_{\mathrm{col}} - d_B), \tag{80}$$

where η' is the mean free path of the source particle in the new zone.

When a source particle is scattered a new direction μ' is chosen uniformly at random from $p(\mu, \mu')$, the Thomson phase function integrated over azimuth. The quantity $p(\mu, \mu')$ is normalized such that

$$\int_{-1}^{+1} p(\mu, \mu')\,\mathrm{d}\mu' = \int_{-1}^{+1} p(\mu', \mu)\,\mathrm{d}\mu = 1 \tag{81}$$

with

$$p(\mu, \mu') = p(\mu', \mu), \tag{82}$$

where

$$p(\mu, \mu') = \tfrac{3}{16}[(3 - \mu^2) + (3\mu^2 - 1)\,\mu'^2]. \tag{83}$$

To obtain μ' uniformly at random from the $p(\mu, \mu')$ distribution for a given μ, we solve for x in the equation

$$2\int_0^x p(\mu, \mu')\,\mathrm{d}\mu' = r, \tag{84}$$

where r is a uniform random number between 0 and 1. This equation reduces to

$$\tfrac{1}{8}(3\mu^2 - 1)\,x^3 + \tfrac{3}{8}(3 - \mu^2)\,x - r = 0 \tag{85}$$

and may be solved for real values of x by standard methods. The derived value of μ' may be either positive or negative. A uniform random number r between 0 and 1 is chosen to make the decision. If

$$r \geqslant 0.5, \quad \mu' = x. \tag{86}$$

If

$$r < 0.5, \quad \mu' = -x. \tag{87}$$

The source particles of each species are followed through the atmosphere until either, they escape from the top of the atmosphere into interstellar space, collide with the totally absorbing lower-base surface, or have their weights drop to a very small fraction of their original values. If a source particle reaches either the top or the bottom of the atmosphere during transfer, its history is terminated and the energy it is carrying is permanently lost to the atmosphere. When its current weight drops below ω_{LIMIT} the remaining energy of the particle is absorbed at its current location in the atmosphere. The choice of ω_{LIMIT}, the weight limit, is made somewhat arbitrarily. It was decided primarily on the basis of practical considerations, as discussed in the following section on the results of a trial calculation. A tally is kept of the amount of energy deposited in each zone of the atmosphere by each species of source particle. In the case of the continuum source particles the tallied total amount of energy absorbed in a given zone of thickness $\Delta z'$, for a particular species of particle associated with wavelength λ, is equal to $4\pi K'_\lambda J_\lambda \Delta z'$. In the case of a particular species of bound-bound source particle the tallied amount of energy absorbed in the same zone is equivalent to

$$4\pi \Delta z' \int_{-\infty}^{+\infty} \frac{K_{\lambda \text{BB}}}{K_\lambda} \cdot K'_\lambda J_\lambda \, \mathrm{d}(\Delta\lambda).$$

4. Results

The Monte Carlo relaxation method has been applied to the computation of a model atmosphere for a pure hydrogen early-type star. The stellar mass was taken as 15 $M_\odot$, and the radius as 6 $R_\odot$, giving a surface gravity g of 1.14×10^4 cm sec^{-2}. Lower-base boundary conditions of $T_0 = 50000$ K and $\rho_0 = 5.0 \times 10^{-8}$ grms cm^{-3} were selected. These boundary conditions were chosen so that a model atmosphere with approximately 20 zones would be an adequate representation of a real early-type stellar atmosphere to include both optically thick and optically thin regions. For practical reasons an 18-zone model was finally adopted. Experience showed that the scarcity of photon-matter interactions in the optically thin outer zones may cause difficulty in the reliable determination of their physical states. To reduce the likelihood of such an occurrence the outermost zones were taken to be wider than the lower zones. The quantity $\log_{10}(p_i/p_{i+1})$ was taken as 0.4, 0.6, and 1.0 for zones 16, 17, and 18, respectively.

The number of source particles of each species originating in each zone, and the weight limit associated with each species of particle, critically determine whether or not the Monte Carlo relaxation technique may successfully be used to compute a model stellar atmosphere. For the lower base boundary n_B was taken as 2000 for each species of particle. For each of the lower zones 1–15, n_z was taken as 2000 for each species of source particle. For the outermost zones 16, 17, and 18, n_z was taken to be larger by factors up to 2.5 to reduce the chance of substantial fluctuations occurring in the amount of radiation absorbed at each wavelength in these zones.

A total of nearly two million source particles were followed in the solution of the radiative transfer problem during each iteration of the atmosphere. Practical considerations prevented any significantly larger number of source particles from being used. The weight limit, ω_{LIMIT}, also was chosen somewhat arbitrarily from practical considerations. It was set equal to 0.005 ω_0, or 0.5% of the original weight of the particle.

If substantial statistical fluctuations occur in the amount of energy absorbed at each wavelength, in any given zone, the possibility exists of oscillations in the electron temperature progressively building into an instability during successive iterations. To avoid the danger of instability n_B and n_z must be large while ω_{LIMIT} must be small. Experience showed that with the above choices of these parameters temperature instabilities could occur at large and small optical depths after the fourth iteration from the isothermal L.T.E. state. However, with the available computation facilities (CDC 3200) it was not feasible to improve the choices of the n_B, n_z, and ω_{LIMIT} parameters substantially. The significance of the particular choices of these parameters for each species of source particle will be discussed further in the following section.

To study the statistical fluctuations in the atomic level populations over many iterations of the atmosphere, it was necessary to avoid temperature instabilities. Three kinds of artificial damping were applied during each iteration so that the instability problem would not occur. These are:

(i) Each successively higher and more tenuous zone was not permitted to have a temperature greater than that of the zone immediately below it.

(ii) No zone was permitted to acquire an electron temperature greater than that of a black body which would emit the same total amount of energy per cm^3 per second as was absorbed by the zone material. This condition ensured temperature stability in the deeper optically thick zones.

(iii) To ensure stability in the outermost two or three optically thin zones the temperature of each zone was not permitted to be greater than that obtained from the previous iteration.

Application of each or any of these three types of damping risks possible overdamping of the temperature profile of the atmosphere. The outer zones might perhaps become too cool because of unusually large downward fluctuations of temperature occurring in the deeper zones. It should be borne in mind also that very recent calculations by FEAUTRIER (1968) indicate that constraints (i) and (iii) will become inapplicable at very small optical depths. Here non-L.T.E. effects become significant and cause a rise in temperature with decreasing optical depth. The temperature profile obtained for the atmosphere by making use of these artificial damping devices did not differ noticeably from the profile obtained without any damping. This point will be discussed further below.

The relaxation of the atmosphere from an initial non-equilibrium isothermal L.T.E. state to a stabilized non-L.T.E. state proceeded extremely rapidly. No more than three iterations were required to obtain stabilization, each iteration taking

TABLE I

Model atmosphere results. Physical parameters

Zone No.	T_e (K)	ρ grms cm^{-3}	Δx (cm)	$\tau_{4000Å}$	N_e (cm^{-3})	b_1	b_2	b_3	b_4	b_5	b_6
1	48860.8	3.955E−8	3.372E+8	1.692E+3	2.382E+16	1.116E+0	9.220E−1	9.369E−1	9.372E−1	9.418E−1	1.0001
2	48860.8	2.486E−8	3.390E+8	6.872E+2	1.497E+16	1.051E+0	9.292E−1	9.462E−1	9.481E−1	9.519E−1	1.0001
3	48860.8	1.562E−8	3.410E+8	2.806E+2	9.408E+15	1.001E+0	9.324E−1	9.515E−1	9.545E−1	9.579E−1	1.0001
4	48860.8	9.809E−9	3.430E+8	1.131E+2	5.909E+15	9.669E−1	9.337E−1	9.547E−1	9.586E−1	9.618E−1	1 0001
5	48844.4	6.170E−9	3.447E+8	4.694E+1	3.717E+15	9.402E−1	9.328E−1	9.556E−1	9.601E−1	9.633E−1	1.0001
6	48844.4	3.894E−9	3.451E+8	2.111E+1	2.346E+15	9.303E−1	9.378E−1	9.625E−1	9.673E−1	9.704E−1	1.0000
7	45202.5	2.640E−9	3.219E+8	1.023E+1	1.590E+15	7.647E−1	9.732E−1	9.893E−1	9.920E−1	9.938E−1	1.0000
8	40928.9	1.831E−9	2.932E+8	5.142E+0	1.103E+15	5.297E−1	9.411E−1	9.707E−1	9.754E−1	9.785E−1	1.0000
9	35198.0	1.339E−9	2.534E+8	2.650E+0	8.065E+14	2.541E−1	7.838E−1	8.399E−1	8.568E−1	8.653E−1	1.0000
10	30169.0	9.779E−10	2.192E+8	1.368E+0	5.892E+14	1.129E−1	6.543E−1	7.370E−1	7.646E−1	7.780E−1	1.0001
11	26538.0	6.959E−10	1.946E+8	6.918E−1	4.193E+14	5.512E−2	5.791E−1	6.857E−1	7.205E−1	7.373E−1	1.0001
12	23367.1	4.942E−10	1.733E+8	3.374E−1	2.978E+14	2.460E−2	4.974E−1	6.421E−1	6.852E−1	7.061E−1	1.0001
13	21253.6	3.406E−10	1.588E+8	1.623E−1	2.052E+14	1.278E−2	4.285E−1	6.103E−1	6.602E−1	6.847E−1	1.0001
14	20481.8	2.223E−10	1.538E+8	7.707E−2	1.340E+14	1.054E−2	3.672E−1	5.699E−1	6.233E−1	6.497E−1	1.0001
15	20481.8	1.404E−10	1.539E+8	3.818E−2	8.460E+13	1.190E−2	3.547E−1	5.369E−1	5.921E−1	6.193E−1	1.0001
16	17556.7	8.775E−11	2.537E+8	1.682E−2	5.287E+13	2.891E−3	1.837E−1	3.138E−1	3.703E−1	4.006E−1	1.0001
17	11766.9	4.350E−11	2.544E+8	4.201E−3	2.620E+13	2.350E−5	2.542E−2	6.573E−2	9.497E−2	1.144E−1	1.0056
18	6880.7	1.481E−11	2.447E+8	8.520E−4	8.918E+12	7.744E−8	4.316E−2	1.152E−1	5.913E−1	1.121E+0	8.1807

approximately 200 min on a CDC 3200 computer. After stabilization any variations in the results from one iteration to the next were statistical fluctuations due to the nature of the Monte Carlo technique. The question of convergence will be discussed in the following section. The main results of the computation are given in Tables I and II.

Table I gives the values of the basic physical parameters for each zone averaged over 10 consecutive iterations after stabilization. Possible oscillations in the temperature profile were damped during successive iterations. After stabilization the profile remained essentially constant to within a few tens of degrees Kelvin. Column 1 gives the zone number, zone 1 being the deepest and densest immediately adjacent to the lower-base boundary, and zone 18 being the highest and most tenuous immediately adjacent to interstellar space. Column 2 gives the electron temperature, T_e, in degrees Kelvin. Column 3 gives the density, ρ, in grms cm^{-3}. Column 4 gives the thickness of each zone, Δx, in cms. Column 5 gives $\tau_{4000\,\text{Å}}$, the optical depth at 4000 Å for the center of each zone. Column 6 gives the electron number density, N_e, in cm^{-3}. Columns 7 through 12 give b_n, the departures of the atomic level populations from their corresponding L.T.E. values, for levels of principal quantum number 1–5 and for the continuum labelled level 6. The quantity b_n is defined by

$$b_n = \frac{N_{n\,\text{Non-LTE}}}{N_{n\,\text{LTE}}}, \tag{88}$$

where N_n is the number density, in cm^{-3}, for level n.

TABLE II

Model atmosphere results. Statistical errors

Zone No.	$\Delta\rho/\rho$	$\Delta(\Delta x)/\Delta x$	Δb_1	Δb_2	Δb_3	Δb_4	Δb_5	Δb_6
1	6.331E − 3	6.254E − 3	1.0167	1.0062	1.0053	1.0051	1.0049	1.0000
2	5.632E − 3	1.104E − 2	1.0135	1.0058	1.0048	1.0045	1.0044	1.0000
3	6.289E − 3	1.372E − 2	1.0107	1.0056	1.0046	1.0043	1.0041	1.0000
4	4.268E − 3	1.446E − 2	1.0093	1.0054	1.0044	1.0041	1.0040	1.0000
5	2.086E − 2	1.506E − 2	1.0090	1.0056	1.0046	1.0043	1.0041	1.0000
6	1.728E − 3	1.645E − 2	1.0072	1.0042	1.0034	1.0032	1.0030	1.0000
7	6.943E − 3	2.233E − 2	1.0354	1.0199	1.0169	1.0155	1.0148	1.0000
8	4.824E − 3	3.136E − 2	1.0292	1.0170	1 0161	1.0147	1.0140	1.0000
9	3.571E − 4	3.986E − 2	1.0302	1.0368	1.0325	1.0293	1.0277	1.0000
10	8.476E − 4	4.580E − 2	1.0420	1.0559	1.0516	1.0462	1.0437	1.0000
11	1.154E − 3	5.032E − 2	1.0491	1.0585	1.0616	1.0549	1.0517	1.0000
12	1.200E − 3	5.499E − 2	1.0553	1.0586	1.0726	1.0643	1.0613	1.0000
13	1.932E − 3	5.811E − 2	1.0543	1.0424	1.0693	1.0610	1.0569	1.0000
14	1.392E − 3	5.798E − 2	1.0565	1.0437	1.0698	1.0625	1.0587	1.0000
15	1.419E − 3	5.626E − 2	1.0661	1.0605	1.0831	1.0726	1.0675	1.0000
16	2.310E − 3	3.237E − 2	1.0857	1.0918	1.1192	1.1053	1.0981	1.0000
17	4.577E − 3	2.882E − 2	1.1396	1.1838	1.2213	1.1966	1.1815	1.0000
18	6.948E − 3	2.655E − 2	1.2189	1.2932	1.3040	1.2676	1.2415	1.0035

Table II gives the statistical errors of the results in Table I. Column 1 gives the zone number as in Table I. Column 2 gives $\Delta\rho/\rho$, where $\Delta\rho$ is the standard error of ρ, the arithmetic mean of the density for each zone. Column 3 gives $\Delta(\Delta x)/\Delta x$, where $\Delta(\Delta x)$ is the standard error of Δx, the arithmetic mean of the width of each zone. Columns 4–9 give Δb_n, the standard errors of the geometrical means, b_n, of the departures from L.T.E. To avoid confusion in the interpretation of Δb_n it should be pointed out that the standard error of the geometrical mean, $\sigma(\bar{y}_{GM})$, is defined here to be

$$\sigma(\bar{y}_{GM}) = \text{ANTILOG}\left\{\sqrt{\sum_{i=1}^{m} \frac{[\log_{10}(y_i) - \log_{10}(\bar{y}_{GM})]^2}{m(m-1)}}\right\}, \tag{89}$$

where $\bar{y}_{GM}$ is the geometrical mean of y, and m is the number of values of y on which $\bar{y}_{GM}$ is based.

The uncertainty in the temperature of each zone was obtained from the results of four successive iterations, made after stabilization of the temperature profile, in each of which random oscillations in the temperature of each zone were not damped in any way. The mean temperature profile remained close to that obtained when the profile was damped, within the range of the statistical temperature fluctuations between successive iterations. For zones 1–5 the standard error in T_e is close to 250 K, reaching 500 K in zone 7. For zones 8 and 9 the error is approximately 750 K, reaching 1000 K in zone 10. For zones 11–18 the error is approximately 1500 K.

To avoid possible confusion the following examples illustrate the notation used in Tables I and II:

$$3.955\ \text{E} - 8 = 3.955 \times 10^{-8}$$
$$3.372\ \text{E} + 8 = 3.372 \times 10^{8}$$
$$1.116\ \text{E} + 0 = 1.116\,.$$

5. Discussion

Non-L.T.E. effects in the level populations of the hydrogen atom in early-type stellar atmospheres have been studied by MIHALAS (1967b, c). The physical theory he used differs in some details from that described in Section 2. In particular there are differences in the assumed chemical composition, the model of the hydrogen atom, the treatment of the statistical equilibrium equations, the formulation of the source function, and the determination of the local temperature.

MIHALAS (1967b) has computed a model for an effective temperature T_{eff} of 25000 K, and surface gravity g of 10^4 cm sec^{-2}. The atomic model for hydrogen was approximated with 15 bound levels and the continuum. The statistical equilibrium equations were solved for the first 10 levels with the remaining levels $n=11$ through $n=15$ assumed to be in L.T.E. Departure coefficients, d_n, were calculated for the lowest 3 levels. The quantity d_n is related to b_n by

$$d_n = b_n - 1\,. \tag{90}$$

The results show that below an optical depth $\tau_{4000\,\text{Å}} \simeq 2 \times 10^{-2}$ all the level populations are very close to their L.T.E. values. Higher in the atmosphere departures from L.T.E. occur. Level $n=1$ becomes overpopulated, while level $n=2$ becomes somewhat depopulated. The quantity d_1 is approximately equal to unity near $\tau_{4000\,\text{Å}} \simeq 10^{-4}$, while $d_2 \simeq -0.3$ at the same optical depth. The quantity d_3 remains close to zero. MIHALAS (1967c) has extended this work by improving the treatment of the transfer of the Lyman continuum and computed two more models for effective temperatures of 20000 K and 25000 K. Both refer to surface gravities of 10^4 cm sec^{-2}. For a T_{eff} of 25000 K the results obtained are similar to those in the earlier paper. For a T_{eff} of 20000 K the level populations are very close to L.T.E. below an optical depth $\tau_{4000\,\text{Å}} \simeq 5 \times 10^{-3}$. Higher in the atmosphere deviations from L.T.E. occur. The lowest level $n=1$ becomes overpopulated with $d_1 \simeq 4$ at $\tau_{4000\,\text{Å}} \simeq 10^{-5}$, and level $n=2$ becomes somewhat depopulated with $d_2 \simeq -0.4$ at the same optical depth. The reliability of the results obtained by the trial application of the relaxation method may be checked by comparison with the results obtained by Mihalas. The latter results have been obtained by methods of proven reliability.

The results presented in Table I have been plotted in Figures 1, 2, and 3. The main features of the electron temperature and density profiles are shown in Figure 1. The apparent departures of the level populations from L.T.E., as a function of optical depth $\tau_{4000\,\text{Å}}$, are shown in Figures 2 and 3. Table II shows the stability of the solution for the atomic level populations. The stability of the temperature profile has been discussed in the previous section.

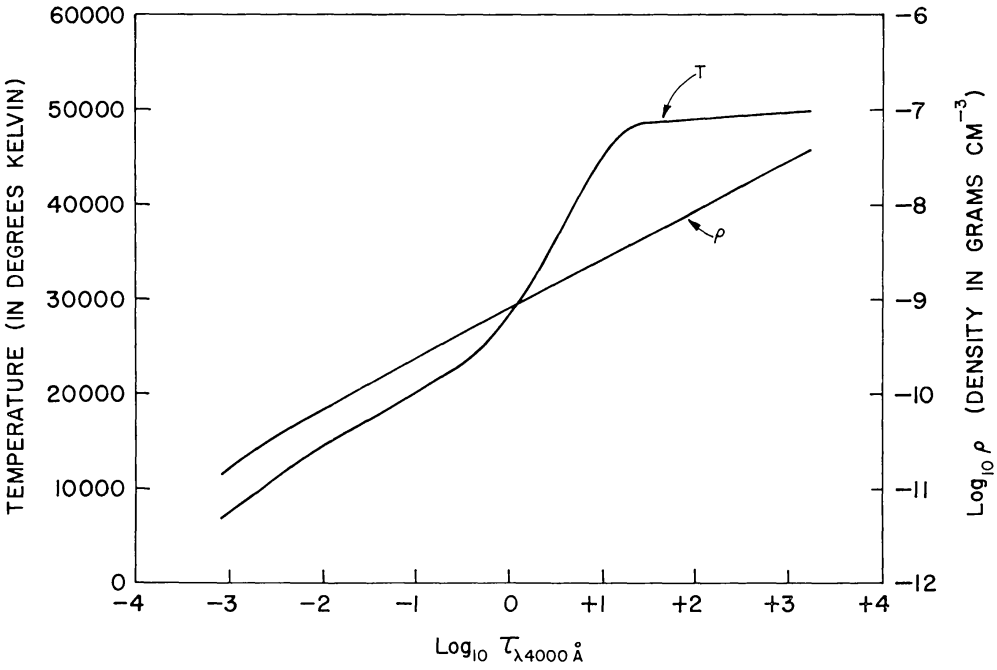

Fig. 1. Electron temperature and density profiles for a pure hydrogen early-type model atmosphere. Boundary conditions were chosen as $T_0 = 50000$ K, $\rho_0 = 5.0 \times 10^{-8}$ grms cm^{-3}.

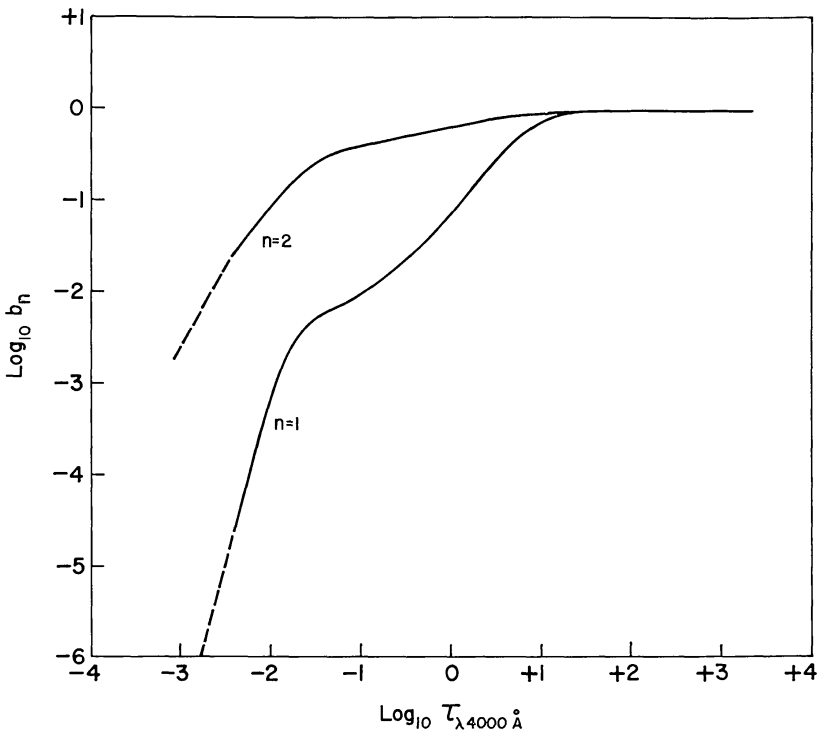

Fig. 2. Apparent departures, b_n, from L.T.E. for the hydrogen atom for principal quantum numbers $n = 1$ and $n = 2$.

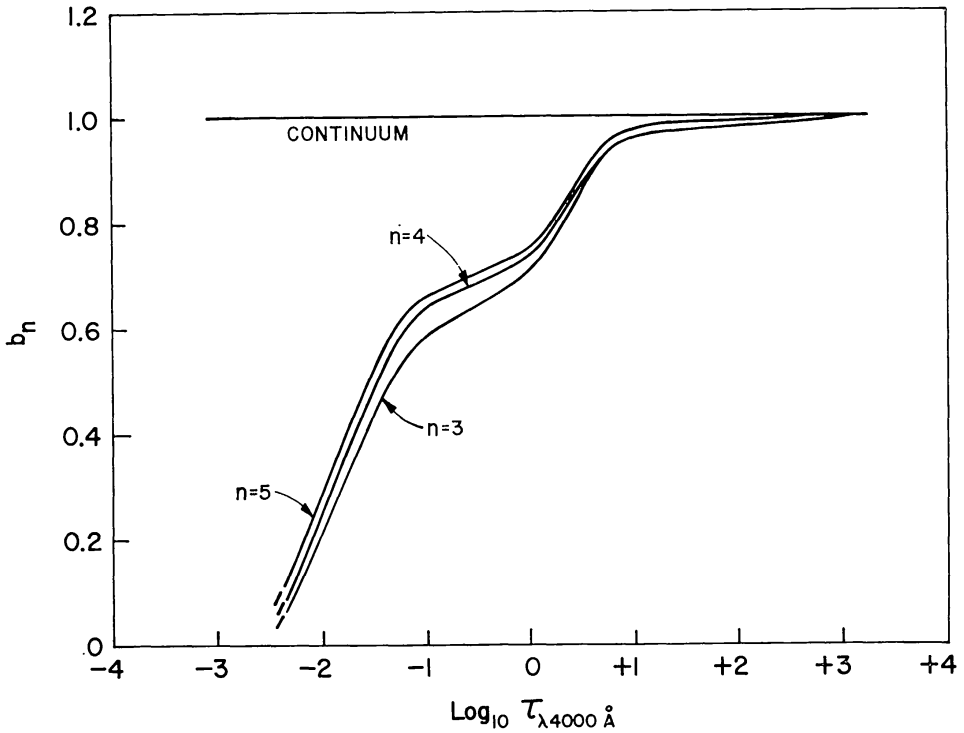

Fig. 3. Apparent departures, b_n, from L.T.E. for the hydrogen atom for principal quantum numbers $n = 3, 4, 5$ and for the continuum.

The temperature profile shown in Figure 1 requires some explanation because of its unusual behavior at large optical depths. It indicates that for optical depths, $\tau_{4000\,\text{Å}}$, greater than about 20 the model atmosphere is unable to cool from its initial isothermal state. This implies that the net outward flux of radiation becomes zero at such large depths. The reason is the breakdown of the Monte Carlo technique. At large optical depths the upward and downward radiation fluxes, F_+ and F_- respectively, are large. However, the net outward flux given by

$$\Delta F = F_+ - F_- \tag{91}$$

is relatively small. Because of the limited number of source particles which must be used to transfer the radiant energy, small fluctuations in F_+ and F_- can easily occur and be larger than ΔF which will then become indeterminate. At smaller optical depths, while ΔF should remain the same as before, both F_+ and F_- are smaller and $\Delta F/F$ is larger. In this case fluctuations in F_+ and F_- have much less effect on the determination of ΔF. This qualitative explanation may be put on a quantitative basis by considering the value of the parameter n_z and the optical thicknesses of the deepest zones of the atmosphere.

Consider the deepest zone immediately adjacent to the lower-base boundary. For a temperature of 50000 K with the zone in L.T.E. the optical thickness, $\Delta\tau$, in each of the bound-free continua is of the order of 10^3. A total of n_z source particles of each species originate uniformly at random throughout the thickness of the zone. No source particle of a given species should originate at an optical distance less than about $\Delta\tau/n_z$ from either of the zone boundaries. The direction of emission is chosen uniformly at random from an isotropic distribution. The particle originating closest to either of the zone boundaries may be expected to travel an optical distance of about $(\Delta\tau/n_z)^2$ before crossing into the adjacent zone. Each source particle may be expected to suffer substantially complete absorption by the stellar material within an optical distance of the order of unity from its point of origin. Consequently, if

$$\{\Delta\tau/n_z\}^2 \gtrsim 1 \tag{92}$$

none of the information carried by the source particles originating in that zone can leak into the adjacent zones. As a result the zone cannot cool because the net outward flux is zero. In the trial calculation n_z was set equal to 2000. With $\Delta\tau \sim 10^3$ in the deepest layers of the atmosphere Equation (92) shows that the first few zones above the lower base boundary will be unable to cool. The reliable determination of ΔF will be discussed further below.

Comparison of the apparent departures from L.T.E., shown in Figures 2 and 3, with the results obtained by MIHALAS (1967b, c) show that although our solution has stabilized it is still a *long* way from being physically realistic. The apparent departures from L.T.E. remain far from small even at large optical depths. Stabilization of the solution after only 3 iterations was rather surprising particularly in view of the apparent rapid relaxation towards the physically realistic solution manifest in the initial few iterations. During the first few iterations the ground level in the outermost

zone increased in population by a factor of about 3 from one iteration to the next as the temperature dropped and recombination from the continuum occurred. Such a large initial rate of relaxation was extremely encouraging and suggested that a converged solution could be obtained with perhaps 20 or 30 iterations. However, these initial hopes were not fulfilled because of the occurrence of unacceptably large fluctuations in the solution at large optical depths. These fluctuations severely adversely affect the solution at smaller depths. The essential problem encountered is that ΔF is not being accurately maintained constant with optical depth. In particular ΔF is uncertain at large optical depths where its accurate evaluation is most difficult. The solution to the problem of maintaining flux constancy to high accuracy is to select the parameters n_B, n_z, and ω_{LIMIT} on the basis of the following considerations.

Consider again a typical zone deep in the atmosphere near the lower-base boundary. At each wavelength the upward and downward fluxes of radiation are represented by approximately $n_z/2$ source particles. If it is assumed that each of these source particles eventually crosses one or the other of the zone boundaries before thermalization the quantities F_+ and F_- at either boundary are represented by $(n_z/2)\pm\sqrt{(n_z/2)}$source particles. Consequently ΔF cannot be known to a fractional accuracy better than about $2/\sqrt{n_z}$. All the source particles of a particular species will reach either one of the zone boundaries only in the limit of small optical thickness. In practice the optical thickness of a zone at some, or all, wavelengths may be very far from small. To ensure that each of the source particles reaches either boundary before thermalization a suitable choice of ω_{LIMIT} must be made for each wavelength by considering the optically thickest zone.

For a typical source particle which originates near the center of a zone of optical thickness $\Delta\tau$ the optical path it must traverse to reach one of the boundaries will be of the order of $(\Delta\tau/2)^2$. If ω_{LIMIT} is so chosen that

$$\frac{\omega_{\text{LIMIT}}}{\omega_0} \lesssim \exp\left\{-\left[\frac{\Delta\tau}{2}\right]^2\right\} \tag{93}$$

all the source particles will reach either of the boundaries before thermalization and be included in the determination of ΔF at each boundary.

With currently available methods for the computation of model stellar atmospheres it is possible to maintain ΔF to an accuracy of better than 0.1%. To use the Monte Carlo relaxation technique to obtain ΔF to the same accuracy a value of n_z of the order of 2×10^6 is demanded. This would be an increase of a factor 10^3 compared with the value of n_z used in the trial calculation. Choosing sufficiently small values of the parameter ω_{LIMIT} so that the same flux constancy could be maintained for all continuum wavelengths, and for the lines, would also be a problem. In particular the accurate transfer of the Lyman continuum and the Lyman lines would be very difficult. As the relaxation from a high-temperature isothermal state proceeds, the lowest bound levels in the outermost zones of the atmosphere become increasingly populated by recombination from the continuum. In particular the population of

the ground state increases very markedly and as a result the zones become increasingly optically thick to the Lyman continuum and Lyman lines. The somewhat arbitrary but necessary choice of ω_{LIMIT} as equal to 0.005 ω_0 prevents the migration of a source particle further than an optical distance of the order of 5.3 from its point of origin. The parameter ω_{LIMIT} should ideally be chosen using the condition given in Equation (93). To avoid changing ω_{LIMIT}, but still maintaining the same flux accuracy, an alternative procedure would be to decrease the zone thickness in accordance with the same condition. Choice of a large value for n_z(and n_B), and an appropriately small value of ω_{LIMIT} for each wavelength, would enable the temperature profile of the atmosphere to be very reliably determined. There would be no need to resort to artificial damping procedures to maintain stability in the temperature profile.

In conclusion, the Monte Carlo relaxation method shows future promise as a very simple technique for the computation of model stellar atmospheres. However, more accurate and detailed investigations of the convergence properties of the method are required before it can be applied to the interpretation of stellar spectra. Continued development of the method will require a substantial increase in the speed of the available electronic computing machines.

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